Global Theory of Quantum Boundary Conditions and Topology Change

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Abstract

We analyze the global theory of boundary conditions for a constrained quantum system with classical configuration space a compact Riemannian manifold M with regular boundary $\Gamma = \partial M$. The space \mathcal{M} of self-adjoint extensions of the covariant Laplacian on M is shown to have interesting geometrical and topological properties which are related to the different topological closures of M. In this sense, the change of topology of M is connected with the non-trivial structure of \mathcal{M} . The space \mathcal{M} itself can be identified with the unitary group $\mathcal{U}(L^2(\Gamma,\mathbb{C}^N))$ of the Hilbert space of boundary data $L^2(\Gamma,\mathbb{C}^N)$. This description, is shown to be equivalent to the classical von Neumann's description in terms of deficiency index subspaces, but it is more efficient and explicit because it is given only in terms of the boundary data, which are the natural external inputs of the system. A particularly interesting family of boundary conditions, identified as the set of unitary operators which are singular under the Cayley transform, $\mathcal{C}_{-} \cap \mathcal{C}_{+}$ (the Cayley manifold), turns out to play a relevant role in topology change phenomena. The singularity of the Cayley transform implies that some energy levels, usually associated with edge states, acquire an infinity energy when by an adiabatic change the boundary conditions reaches the Cayley submanifold \mathcal{C}_{-} . In this sense topological transitions require an infinite amount of quantum energy to occur, although the description of the topological transition in the space \mathcal{M} is smooth. This fact has relevant implications in string theory for possible scenarios with joint descriptions of open and closed strings. In the particular case of elliptic self-adjoint boundary conditions, the space \mathcal{C}_{-} can be identified with a Lagrangian submanifold of the infinite dimensional Grassmannian. The corresponding Cayley manifold \mathcal{C}_{-} is dual of the Maslov class of \mathcal{M} . The phenomena are illustrated with some simple low dimensional examples.

1. Introduction

The analysis of the role of the boundary of quantum systems has became a recent focus of activity in different branches of physics which range from the analysis of edge states in the Hall effect [1] to quantum black hole physics [2][3], quantum gravity [4], cosmology [5], strings, D-branes [6] and M-theory (see [7] for a review). In QFT the relevance of boundary conditions is also crucial for phenomena like spontaneous breaking of symmetries, anomalies [8], the Casimir effect [9] or the analysis of the anysotropic structure of the cosmic background radiation [10].

The conservation of probability in quantum mechanics, which is intrinsically connected with the unitarity principle, imposes severe constraints on the boundary behaviour of quantum states in systems evolving in bounded domains. The analytical condition, which is encoded by selfadjointness of the hamiltonian operator, contains all the quantum subtleties associated to the unitary principle and the dynamical behaviour at the boundary. In the classical field physics there are not so stringent conditions and the classification of the different types of boundary conditions is basically based on phenomelogical considerations rather than in basic physical principles. The existence of a boundary generically enhances the genuine quantum aspects of the system. Famous examples of this behaviour are Young slit experiments and the Aharanov-Bohm effects, which pointed out the relevance of boundary conditions in the quantum theory. Another examples of quantum physical phenomena which are intimately related to boundary conditions are the Casimir effect [11], the role of edge states [12] and the quantization of conductivity [13] in the quantum Hall effect. The physics of boundary conditions is becoming very relevant in quantum gravity, string theory and brane theory. Effects like topology change [14], quantum holography [4][15] and AdS/CFT correspondence [16] show the relevance of boundaries in the description of fundamental physical phenomena. Moreover, the recent observation of a suppression of quadropole and octopole components of the cosmic background radiation might be connected with the boundary conditions or the space topology of the Universe [10]. To some extent the role of boundary phenomena has been promoted from academic and phenomelogical simplifications of more complex physical systems to a higher status connected with very basic fundamental principles.

Another kind of interesting applications arise in pure mathematics in the study of the index theorem for manifolds with boundary [17].

The dynamics of a system with boundary requires information about the physical properties of the boundary. The boundary conditions macroscopically encode the microscopic or fundamental structure of the material medium that the physical boundary is made off. In fact the dynamics is not well defined until the boundary conditions are not completely specified. In classical mechanics, boundary conditions determines the evolution of the system after reaching the boundary. The corresponding boundary conditions are essentially local, except for those which correspond to the folding of the boundary and lead to non-trivial topology changes across the boundary. In classical field theory boundary conditions are specified by the values of the fields and some of its derivatives necessary to solve the corresponding boundary value problem. In quantum field theories the fluctuations of the bosonic fields, both in the bulk and the boundary, can contribute to the dynamics of the system for open boundary conditions, although the nature of the boundary might require more specific boundary conditions. For fermionic fields boundary conditions are also needed to guarantee the consistency of the theory. In gauge theories, quantum gravity or string theories, however, a more general type of boundary conditions have to be considered to describe the sum over different space-time topologies.

In this paper we consider the global theory of boundary conditions which are compatible with the fundamental properties of a elementary quantum system which is confined on a bounded domain with boundary. From a physical point of view the boundary conditions are determined by the nature of the Hamiltonian in the interior of the domain and by the physical characteristics of the boundary. We analyze the minimal requirements that the quantum theory imposes on boundary conditions in terms of constraints on the values of boundary data, and find out all possible solutions compatible with unitarity. Among all these boundary conditions one finds those which correspond to topological foldings of the boundary, sticky conditions which enhance the role of edge states, and all kind of classical boundary conditions. The space of all these boundary conditions \mathcal{M} exhibit very interesting geometrical and topological structures. It has a group structure and can be identified with an infinite dimensional Grassmannian manifold. The global properties of \mathcal{M} might be relevant for quantum gravity where one has to sum over a very large class of boundary conditions. The study of such a global properties of \mathcal{M} and its connection with the appearance of edge states and topology change is the main motivation of this paper. We identify all conditions involving topology change as a Cayley submanifold of the space of all boundary conditions. We point out the existence of a connection between topology change and the existence of edge states with very large negative energies.

We also analyze the connection of this submanifold with the non-trivial topology of \mathcal{M} and the Maslow index of the grasssmanian structure.

In Sect. 2 we derive a description of quantum boundary conditions in terms of constraints on the boundary data. The equivalence with the classical von Neumann's description in shown in Sect. 3. In Sect. 4 we analyze the geometrical structure of the space of quantum boundary conditions and in Sect. 5, its relation with the infinite dimensional Grassmannian and the two Cayley submanifolds. Finally, the appearance of edge states for boundary conditions in the vicinity of one of the two Cayley submanifolds and its connection with topology changes is discussed in Sect. 6.

2. Quantum Boundary Conditions

Let us consider a non-relativistic point-like particle moving on an n-dimensional orientable compact Riemannian manifold (M,g) with smooth boundary $\Gamma = \partial M$, under the action of a a smooth potential V and a gauge field A defined in a hermitian vector bundle E over M of rank N.

The space of physical states is defined by the completion of the space of smooth sections $C^{\infty}(M, E)$ of E with respect to the norm $\|\cdot\|_2$ induced by the hermitian product

$$\langle \psi_1, \psi_2 \rangle = \int_M (\psi_1(x), \psi_2(x))_x \, d\mu_g(x),$$
 (2.1)

where $d\mu_g(x)$ denotes the Riemannian volume form defined by the orientation of M and the metric g, and $(.,.)_x$ is the hermitian product of E at x. In local coordinates, $d\mu_g(x) = \sqrt{g} d^n x$. The space $L^2(E)$ of physical states contains also non-smooth sections and in fact is independent of the vector bundle E considered and can therefore be identified with $L^2(M, \mathbb{C}^N)$ [18].

Solving the operator ordering problem in an appropriate way yields to a quantum Hamiltonian formally given by

$$\mathbb{H} = -\Delta_A + V,\tag{2.2}$$

where $\Delta_A = d_A^{\dagger} d_A$ is the covariant Laplace-Beltrami operator and V is the smooth potential on M^2 . The covariant differential operator $d_A: C^{\infty}(M, E) \to \Omega^1(M, E)$ maps smooth

The theory can be generalized for piecewise smooth boundaries without pathological cone singularities.

 $^{^{2}}$ The role of the potential V in the discussion is subsidiary provided it has not singularities.

sections of E into 1-forms on M with values on E. There is a natural inner product on the space of E-valued 1-forms $\Omega^1(M, E)$ defined as

$$\langle \alpha, \beta \rangle = \int_M (\alpha(x), \beta(x))_x d\mu_g(x),$$

with $(\alpha(x), \beta(x))_x = g^{ij}(x)h^{ab}(x)\alpha_i^a(x)\beta_j^b$ where $h = h^{ab}\sigma_a \otimes \sigma_b$ denotes the metric bundle and $g = g_{ij}dx^i \otimes dx^j$ the riemannian metric. We shall denote by d_A^{\dagger} the adjoint operator of d_A with respect to the Hilbert space structure defined by hermitian product above.

It is obvious that \mathbb{H} is a symmetric operator on $C_0^{\infty}(M, E)$, the space of smooth sections with compact support in the interior of M. However, in general, \mathbb{H} is not even essentially self-adjoint in $L^2(E)$ because the domain $C_0^{\infty}(M, E)$ is too small, although dense in $L^2(E)$. The adjoint operator \mathbb{H}^{\dagger} is given by the extension of \mathbb{H} to the dense subspace $H^2(E)$ of class 2 Sobolev sections of $L^2(E)$ defined by the closure of the space of smooth sections $C^{\infty}(M, E)$ of E with respect to the norm associated to the hermitian product

$$\langle \psi_1, \psi_2 \rangle_2 = \int_M (\psi_1(x), (-\Delta_A + I)\psi_2(x))_x d\mu_g(x).$$
 (2.3)

The obstruction to the self-adjointness of \mathbb{H} is due to the non-trivial structure of the boundary terms, the Lagrange form, appearing in the integration by parts formula

$$\langle \psi_1, \mathbb{H}\psi_2 \rangle = \langle \mathbb{H}\psi_1, \psi_2 \rangle + i\Sigma (\psi_1, \psi_2),$$
 (2.4)

valid for any pair of smooth sections $\psi_1, \psi_2 \in C^{\infty}(M, E)$. The boundary term

$$\Sigma(\psi_1, \psi_2) = i \int_M d\left[(*d_A \psi_1, \psi_2) - (\psi_1, *d_A \psi_2) \right], \tag{2.5}$$

that by Stokes theorem, takes the form

$$\Sigma(\psi_1, \psi_2) = i \int_{\Gamma} j^* \left[(*d_A \psi_1, \psi_2) - (\psi_1, *d_A \psi_2) \right] = i \int_{\Gamma} \left[(\dot{\varphi}_1, \varphi_2) - (\varphi_1, \dot{\varphi}_2) \right] d\mu_{\Gamma}$$
 (2.6)

which only really depends on the boundary values

$$\varphi_i = j^* \psi_i = \psi_i|_{\Gamma} \qquad (i = 1, 2),$$

of ψ_1 and ψ_2 and its oriented covariant normal derivatives $\dot{\varphi}_1, \dot{\varphi}_2$ given by

$$j^*[*d_A\psi_i] = \dot{\varphi}_i \, d\mu_{\Gamma} \qquad (i = 1, 2).$$

We denote by * the Hodge star operator of the orientable Riemannian manifold (M, g), j^* is the pullback along the immersion $j: \Gamma \to M$ and $d\mu_{\Gamma} = i_{\nu}d\mu_{g}$ the volume form induced on the boundary by the bulk volume form $d\mu_{g}$ and the outward normal ν .

The boundary term $\Sigma(\psi_1, \psi_2)$ has a relevant physical interpretation. It measures the net flux of probability across the boundary. If the operator \mathbb{H} has to be self-adjoint this flux must be null: the incoming flux has to be equal to the outgoing flux, because the evolution operator $\exp it\mathbb{H}$ in such a case is unitary and preserves probability. In fact as it was mentioned before, for sections of compact support, $\psi_1, \psi_2 \in C_0^{\infty}(M, E)$, it vanishes, implying that the Laplace-Beltrami operator Δ_A is symmetric in that domain. The different self-adjoint extensions will be defined in linear dense subspaces of $L^2(E)$ containing $C_0^{\infty}(M, E)$ such that the boundary term Σ vanishes.

The classification of the different possible self-adjoint extensions will easily be derived from the cancellation conditions of the boundary term Σ .

Theorem 1: The set \mathcal{M} of self-adjoint extensions of \mathbb{H} is in one-to-one correspondence with the group of unitary operators of $L^2(\Gamma, \mathbb{C}^N)$.

Proof: The boundary term Σ has to vanish in the linear domain of any selfadjoint extension of \mathbb{H} . Thus, any selfadjoint extension is uniquely characterized by a maximal isotropic subspaces of the boundary data space

$$L^2(\Gamma,\mathbb{C}^N)\times L^2(\Gamma,\mathbb{C}^N)=\left\{(\varphi,\dot{\varphi});\varphi,\dot{\varphi}\ \in L^2(\Gamma,\mathbb{C}^N)\right\}$$

obtained from the completion³ of $C^{\infty}(\Gamma, j^*E) \times C^{\infty}(\Gamma, j^*E) = \{(\varphi, \dot{\varphi}); \varphi, \dot{\varphi} \in C^{\infty}(\Gamma, j^*E)\}$ with repect to the pseudo-hermitian product (Lagrange form) defined by (2.6)

$$\Sigma\left((\varphi_1, \dot{\varphi}_1), (\varphi_2, \dot{\varphi}_2)\right) = i \int_{\Gamma} \left[(\dot{\varphi}_1, \varphi_2)_x - (\varphi_1, \dot{\varphi}_2)_x\right] d\mu_{\Gamma}. \tag{2.7}$$

In the space of boundary data there is also an additional hermitian structure given by

$$\langle (\varphi_1, \dot{\varphi}_1), (\varphi_2, \dot{\varphi}_2) \rangle = \langle \varphi_1, \varphi_2 \rangle + \langle \dot{\varphi}_1, \dot{\varphi}_2 \rangle, \tag{2.8}$$

where

$$\langle \varphi_1, \varphi_2 \rangle = \int_{\Gamma} (\varphi_1, \varphi_2)_x d\mu_{\Gamma}$$
 (2.9)

³ This space does not really depends on which vector bundle E we use to define the hermitian product. It only depends on its rank N, i.e. $L^2(E) = L^2(\Gamma, \mathbb{C}^N)$

denotes the hermitian product on $L^2(\Gamma, \mathbb{C}^N)$ defined by the induced Riemannian structure of the boundary. The identification of the maximal isotropic spaces of the space of boundary data becomes easier if we perform the Cayley transform defined by

$$C((\varphi_{1}, \dot{\varphi}_{1}); (\varphi_{2}, \dot{\varphi}_{2})) = ((\phi_{1}^{+}, \phi_{1}^{-}); (\phi_{2}^{+}, \phi_{2}^{-}))$$

$$= ((\varphi_{1} + i\dot{\varphi}_{1}, \varphi_{1} - i\dot{\varphi}_{1}); (\varphi_{2} + i\dot{\varphi}_{2}, \varphi_{2} - i\dot{\varphi}_{2})).$$
(2.10)

This transformation is an isometry with respect to the hermitian structure $\langle .,. \rangle$ but it does not preserve the pseudo-hermitian structure $\Sigma(.,.)$ defined by the boundary terms.

In fact, the Cayley transform maps $\Sigma(.,.)$ into the pseudo-hermitian product $\Sigma_c(.,.)$ given by

$$\Sigma_c \left((\phi_1^+, \phi_1^-), (\phi_2^+, \phi_2^-) \right) = \frac{1}{2} \langle \phi_1^+, \phi_2^+ \rangle - \frac{1}{2} \langle \phi_1^-, \phi_2^- \rangle.$$
 (2.11)

Thus, it is obvious that the maximal isotropic subspaces of Σ in $L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$ are in one–to–one correspondence with the space of unitary operators $\mathcal{U}(L^2(\Gamma, \mathbb{C}^N))$ of the boundary space $L^2(\Gamma, \mathbb{C}^N)$, i.e. any vector of a maximal isotropic subspace is of the form

$$\varphi - i\dot{\varphi} = U(\varphi + i\dot{\varphi}), \tag{2.12}$$

where U is an unitary operator of $L^2(\Gamma, \mathbb{C}^N)$ which is uniquely associated to such a subspace.

With the above characterization, the set of self-adjoint extensions of \mathbb{H} inherits the group structure of the group of unitary operators $\mathcal{U}\left(L^2(\Gamma,\mathbb{C}^N)\right)$. This characterization can be extended for a larger class of differential operators on $E(M,\mathbb{C}^N)$ like Dirac operators ∂_A [19] and higher order differential operators like Δ_A^k (see appendix C) or ∂_A^k . The only change is that the hermitian structure of the boundary data changes as we change of operator (see examples in appendix C for illustration).

There are two natural boundary conditions where the Cayley transform becomes singular: Dirichlet (U = -1) and Neumann (U = 1) boundary conditions. But the group of boundary conditions is much larger. In general, for spaces M of dimension higher than one $\mathcal{U}\left(L^2(\Gamma,\mathbb{C}^N)\right)$ is an infinite dimensional group. There are two particular subsets of $\mathcal{U}\left(L^2(\Gamma,\mathbb{C}^N)\right)$ which give rise to boundary conditions which are very easily expressed in terms of boundary values. They are defined by

$$\varphi = A_{-}\dot{\varphi}; \qquad \dot{\varphi} = A_{+}\varphi \tag{2.13}$$

in terms of hermitian operators A_{\pm} . The fact that they define selfadjoint extensions of \mathbb{H} follows from the unitarity of the following operators

$$U_{\pm} = \pm \frac{1 - iA_{\pm}}{1 + iA_{+}}. (2.14)$$

3. Equivalence with Von Neumann theory of self-adjoint extensions

The theory of selfadjoint extensions of symmetric operators densely defined in Hilbert spaces was developed by von Neumann [20](see also [21] [22]). We shall see that for the operator \mathbb{H} it leads to the same results as the approach developed in the previous sections.

The von Neumann theory is based on two deficiency spaces \mathcal{N}_{\pm} , which are spanned by the zero modes of the operators $\Delta_A^{\dagger} \mp iI$

$$\mathcal{N}_{\pm} = \ker(\Delta_A^{\dagger} \mp i\mathbb{1}). \tag{3.1}$$

The adjoint operator Δ_A^{\dagger} of the covariant laplacian Δ_A is defined on the subspace

$$\mathcal{D} = \overline{\mathcal{D}_0} + \mathcal{N}_+ + \mathcal{N}_-,$$

of $H^2(E)$ of L^2 , which in general is larger that the domain $\mathcal{D}_0 = C_0^{\infty}(M, E)$ of definition of Δ_A . The von Neumann theorem [20] establishes that

Theorem 2 (von Neumann): There exists a one-to-one correspondence between self-adjoint extensions of Δ_A and unitary operators U from \mathcal{N}_+ to \mathcal{N}_- .

Proof: The domain of the self–adjoint extension Δ^U corresponding to the operator U is $\mathcal{D}_U = \overline{\mathcal{D}_0} + (I+U)\mathcal{N}_+$ where the operator Δ^U is defined by

$$\Delta_A^U \psi = \Delta_A \psi_0 - i\xi_+ + iU\xi_+,$$

for any function of the form $\psi = \psi_0 + (I+U)\xi_+$, with $\xi_+ \in \mathcal{N}_+$ and $\psi_0 \in \overline{\mathcal{D}_0}$. The essential idea for the proof is the existence of a one-to-one correspondence between the extensions of the symmetric operator Δ_A and the extensions of its Cayley transform operator

$$\tilde{U} = \frac{\Delta_A - i \, \mathbb{1}}{\Delta_A + i \, \mathbb{1}},$$

defined from $\operatorname{ran}(\Delta_A + i \mathbb{1})$ into $\operatorname{ran}(\Delta_A - i \mathbb{1})$. When, the deficiency subspaces do have the same dimension, it is possible to extend \tilde{U} to an unitary operator defined in the whole

 $L^2(E)$ Hilbert space. The possible different extensions \tilde{U}_U are parametrized by the unitary operators U from $\operatorname{ran}(\Delta_A + i\mathbb{1})^{\perp} = \ker(\Delta_A^{\dagger} - i\mathbb{1})$ into $\operatorname{ran}(\Delta_A - i\mathbb{1})^{\perp} = \ker(\Delta_A^{\dagger} + i\mathbb{1})$. To every such extension we can associate a selfadjoint extension of Δ_A by the inverse Cayley transformation

$$\Delta_A = i \frac{\tilde{U}_U - \mathbb{1}}{\tilde{U}_U + \mathbb{1}},\tag{3.2}$$

which is now well defined on \mathcal{D}_U .

Let us now analyze the direct connection of this theory with the approach developed in the previous sections. This can be achieved in two steps.

First, we remark that unitary operators from \mathcal{N}_{+} into \mathcal{N}_{-} are in one-to-one correspondence with maximal isotropic subspaces of the total deficiency space $\mathcal{H}_{\pm} = \mathcal{N}_{+} \oplus \mathcal{N}_{-}$, with respect to the natural pseudo-hermitian structure of \mathcal{H}_{\pm} defined by

$$\Sigma_{\pm} \left((\psi_1^+, \psi_1^-), (\psi_2^+, \psi_2^-) \right) = 2 \langle \psi_1^+, \psi_2^+ \rangle - 2 \langle \psi_1^-, \psi_2^- \rangle, \tag{3.3}$$

for any pair of vectors $(\psi_1^+, \psi_1^-); (\psi_2^+, \psi_2^-) \in \mathcal{H}_{\pm}$.

The connection between both approaches is established by the map $j_{\pm}^*: \mathcal{H}_{\pm} \to L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$ which applies (ψ_+, ψ_-) into their boundary values $(\phi_+, \phi_-) \equiv (j^*\psi_+ + i\dot{\varphi}_+, j^*\psi_- - i\dot{\varphi}_-)$ in $L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$, with $j^*\psi_{\pm} = \varphi_{\pm}$ and $j^*[*d_A\psi_{\pm}] = \dot{\varphi}_{\pm} d\mu_{\Gamma}$. The map j_{\pm}^* defines a one-to-one correspondence between \mathcal{H}_{\pm} and $L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$ as a consequence of the following lemma.

Lemma: The map j_{\pm}^* establishes an isomorphism between the deficiency space \mathcal{H}_{\pm} and boundary data $L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$.

Proof: The space \mathcal{H}_{\pm} can be identified with the kernel of the operator $\Delta_A^{\dagger 2} + \mathbb{I}$ because of the identity $\Delta_A^{\dagger 2} + \mathbb{I} = (\Delta_A^{\dagger} - i\mathbb{I})(\Delta_A^{\dagger} + i\mathbb{I})$. The map j_{\pm}^* is obviously injective because if two sections ψ_1 , ψ_2 of \mathcal{H}_{\pm} have the same boundary values their difference $\psi_1 - \psi_2$ will have vanishing boundary values, and the only section on the kernel of $\Delta_A^{\dagger 2} + \mathbb{I}$ with vanishing boundary values is the null section $\psi = 0$. To prove that j_{\pm}^* is surjective one has to show that for any boundary value in $(\varphi, \dot{\varphi}) \in L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$ there is a section ψ on \mathcal{H}_{\pm} such that $j^*\psi = \varphi$ and $j^*[*d_A\psi] = \dot{\varphi} d\mu_{\Gamma}$. But this follows from the solution of the boundary value problem for the differential operator $\Delta_A^{\dagger 2} + \mathbb{I}$. There is a unique solution of the equation $(\Delta_A^{\dagger 2} + \mathbb{I})\psi = 0$ with boundary values $j^*\psi = \varphi$ and $j^*[*d_A\psi] = \dot{\varphi} d\mu_{\Gamma}$. The uniqueness of the solution follows from the strict positivity of the selfadjoint operator $\Delta_A^2 + \mathbb{I}$ with Dirichlet-Dirichlet $\varphi = \Delta_A \varphi = 0$ boundary conditions (see appendix C). The existence of the solution of this generalized boundary value problem can be derived

in a similar way to that of second order differential operators [23]. The solution can be explicitly expressed in terms of the boundary values $\varphi, \dot{\varphi}$ by integrals formulas only involving the kernel $G_0(x, y)$ of the selfadjoint extension of $\Delta_A^2 + 1$ with Dirichlet-Dirichlet $\varphi = \Delta_A \varphi = 0$ boundary conditions,

$$\psi(x) = \int_{\Gamma} \varphi(y) j^* \left[*d_A \ \Delta_A G_0(x, y) \right] - \int_{\Gamma} d\mu_{\Gamma}(y) \ \dot{\varphi}(y) \left[\Delta_A G_0(x, y) \right], \tag{3.4}$$

where the covariant differential operators d_A and Δ_A act on the argument y of the functions and $G_0(x,y)$ is the solution of the equation $(\Delta_A^2 + 1) G_0(x,y) = \delta(d(x,y))$ with the boundary conditions $G_0(x,y) = 0$ and $\Delta_A G_0(x,y) = 0$ for any $x,y \in \Gamma$. d(x,y) is the Riemaniann distance defined on M by the metric g. The formula (3.4) provides an explicit expression for the inverse of the map j^{\pm} and completes the proof of the lemma.

The second step is to show that j_{\pm}^* is, in fact, an isometry between $(\mathcal{H}_{\pm}, \Sigma_{\pm})$ and boundary and $(L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N), \Sigma_c)$. Since $\Delta_A^{\dagger} \psi_a^+ = i \psi_a^+$, a = 1, 2, we have that

$$0 = \langle \psi_{1}^{+}, (\Delta_{A}^{\dagger} - i)\psi_{2}^{+} \rangle = \langle \psi_{1}^{+}, \Delta_{A}^{\dagger}\psi_{2}^{+} \rangle - i\langle \psi_{1}^{+}, \psi_{2}^{+} \rangle$$

$$= \langle \Delta_{A}^{\dagger}\psi_{1}^{+}, \psi_{2}^{+} \rangle + i\Sigma_{c}(\phi_{1}^{+}, \phi_{2}^{+}) - i\langle \psi_{1}^{+}, \psi_{2}^{+} \rangle$$

$$= \langle (\Delta_{A}^{\dagger} - i)\psi_{1}^{+}, \psi_{2}^{+} \rangle - 2i\langle \psi_{1}^{+}, \psi_{2}^{+} \rangle + i\Sigma_{c}(\phi_{1}^{+}, \phi_{2}^{+})$$

$$= -2i\langle \psi_{1}^{+}, \psi_{2}^{+} \rangle + i\Sigma_{c}(\phi_{1}^{+}, \phi_{2}^{+}),$$

$$(3.5)$$

i.e.

$$2\langle \psi_1^+, \psi_2^+ \rangle = \Sigma_c(\phi_1^+, \phi_2^+)$$

In the same way we obtain

$$2\langle \psi_1^-, \psi_2^- \rangle = \Sigma_c(\phi_1^-, \phi_2^-)$$

Hence, the product of two elements $(\psi_1^+, \psi_1^-), (\psi_2^+, \psi_2^-) \in \mathcal{H}_{\pm}$, equals that of the corresponding elements $(\phi_1^+, \phi_1^-), (\phi_2^+, \phi_2^-) \in L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$, i.e.

$$\Sigma_{\pm}((\psi_1^+, \psi_1^-), (\psi_2^+, \psi_2^-)) = \Sigma_c((\phi_1^+, \phi_1^-), (\phi_2^+, \phi_2^-)),$$

which establishes the isometric character of j_{\pm}^* . The results can be summarized in the following theorem.

Theorem 3: The boundary value map j_{\pm}^* defines an isomorphism from the Hilbert space of deficiency vectors $(\mathcal{H}_{\pm}, \Sigma_{\pm})$ to the Hilbert space of boundary data

$$(L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N), \Sigma_c).$$

In consequence, the maximal isotropic subspaces of \mathcal{H}_{\pm} are mapped into those of $L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$ and viceversa. Moreover, the unitary operators from \mathcal{N}_+ into \mathcal{N}_- are in one to one correspondence with those of $L^2(\Gamma, \mathbb{C}^N)$. This shows the equivalence between the von Neumann theory and the geometric theory based on boundary data.

4. Selfadjoint extensions, boundary data and Cayley submanifolds

The characterization of selfadjoint extensions of \mathbb{H} in terms of unitary operators of $\mathcal{U}(L^2(\Gamma,\mathbb{C}^N))$, although equivalent to von Neumann characterization, it is more useful for physical applications because it is purely formulated in terms of boundary data. The constraints involved in the definition of the domain of \mathbb{H}^U imply that the boundary values φ , $\dot{\varphi}$ of the functions of such a domain satisfy the condition

$$\varphi - i\dot{\varphi} = U(\varphi + i\dot{\varphi}). \tag{4.1}$$

Generically, the constraint equation can be solved to express $\dot{\varphi}$ as a function of φ

$$\dot{\varphi} = -i\frac{\mathbb{1} - U}{\mathbb{1} + U}\varphi \tag{4.2}$$

or, alternatively, φ as a functions of $\dot{\varphi}$

$$\varphi = i \frac{\mathbb{1} + U}{\mathbb{1} - U} \dot{\varphi}. \tag{4.3}$$

This explicit resolution of the constraint on the boundary data means that unitarity requires that only half of the dynamical data are independent on the boundary.

The equations (4.2)(4.3) are in fact two different expressions of the Cayley transform relating selfadjoint and unitary operators

$$A = -i\frac{1 - U}{1 + U} \qquad A^{-1} = i\frac{1 + U}{1 - U}.$$
 (4.4)

The inverse transformation being also a Cayley transform

$$U = \frac{1 - iA}{1 + iA}.\tag{4.5}$$

It is obvious that A is only well defined if and only if -1 does not belong to the spectrum of U. The existence of A^{-1} requires that the spectrum of U does not contain the unit $1 \notin \sigma(U)$.

The previous considerations show that there is a distinguished set of self-adjoint extensions of \mathbb{H} for which the expression of the boundary conditions defining their domain cannot be reduced to the simple form given by eq. (4.2) or (4.3). These self-adjoint extensions correspond to the cases where ± 1 are in the spectrum of the corresponding unitary operator The Cayley submanifolds \mathcal{C}_{\pm} are the subspaces of self-adjoint extensions which cannot be defined from (4.2) or (4.3) and they can be described equivalently as follows:

$$C_{\pm} = \left\{ U \in \mathcal{U} \left(L^2(\Gamma, \mathbb{C}^N) \right) \mid \pm 1 \in \sigma(U) \right\}. \tag{4.6}$$

Notice that the unitary operators $U = \pm 1$ are in the Cayley submanifolds C_{\pm} , respectively. U = -1 belongs to the Cayley submanifold C_{-} and corresponds to Dirichlet boundary conditions (4.3):

$$\varphi = 0. \tag{4.7}$$

U = 1 is not in the Cayley submanifold C_- but in C_+ and corresponds to the self-adjoint operator A = 0 which defines Neumann boundary conditions

$$\dot{\varphi} = 0. \tag{4.8}$$

There is a formal property which distinguishes the two Cayley submanifolds. The submanifold C_+ has a group structure whereas C_- and thus also $C_- \cap C_+$ does not because the composition is not a inner operation.

5. The self-adjoint Grassmannian

The identification of the space \mathcal{M} with the unitary group of boundary data $\mathcal{U}(L^2(\Gamma,\mathbb{C}^N))$ provides a group structure to the space of selfadjoint realizations of Δ_A . This also shows that it has a non-trivial topological structure. All even homotopy groups vanish $\pi_{2n}(\mathcal{M}) = 0$ but all odd homotopy groups are non-trivial $\pi_{2n+1}(\mathcal{M}) = \mathbb{Z}$ (Bott periodicity theorem). The fact that the first homotopy group $\pi_1(\mathcal{M}) = \mathbb{Z}$ means that the space of boundary conditions is non-simply connected. However the set of selfadjoint

operators in $L^2(\Gamma, \mathbb{C}^N)$ is a topologically trivial manifold. This means that the characterization of selfadjoint extensions of Δ_A by means of the Cayley transform (4.2) or (4.3) cannot provide a global description of \mathcal{M} . In fact, the parametrization (4.5) and its inverse

$$U^{-1} = \frac{\mathbb{1} + iA}{\mathbb{1} - iA}. ag{5.1}$$

can be considered as local coordinates in the charts $\mathcal{M} \setminus \mathcal{C}_{\pm}$ of the space \mathcal{M} of selfadjoint extensions Δ_A . The topology of each chart is trivial but that of \mathcal{M} is highly non-trivial. In this sense, the Cayley submanifold \mathcal{C}_{\pm} intersects all non-contractible cycles of \mathcal{M} .

Since $\pi_0(\mathcal{M}) = 0$ and $\pi_1(\mathcal{M}) = \mathbb{Z}$ the first cohomology group of \mathcal{M} is $H^1(\mathcal{M}) = \mathbb{Z}$. The generator of this cohomology group is given by the first Chern class of the determinant bundle defined over \mathcal{M} . The determinant of infinite dimensional operators U is ill defined and proper definition requires the introduction of an ultraviolet regularization. In particular, it is necessary to restict the boundary conditions to the subspace \mathcal{M}' defined by the unitary U operators of \mathcal{M} which are of the form $U = \mathbb{1} + K$ with K a Hilbert-Schmidt operator (i.e. tr $K^{\dagger}K < \infty$). If $-1 \notin \sigma(U)$ this property of K is equivalent to the requirement that the boundary operator A is also a Hilbert-Schmidt operator. Indeed,

$$K_A = \frac{2A}{i\mathbb{1} - A}, \quad A = \frac{iK_A}{2 + K_A}$$

hence,

$$K_A^{\dagger} K_A = \frac{4A^2}{\mathbb{1} + A^2}, \quad A^{\dagger} A = \frac{K_A^{\dagger} K_A}{(2 + K_A^{\dagger})(2 + K_A)}$$

and

$$\operatorname{Tr} \, K_A^\dagger K_A = 4 \operatorname{Tr} \, \frac{A^2}{\mathbb{1} + A^2} \leq 4 \operatorname{Tr} \, A^2, \quad \operatorname{Tr} \, A^\dagger A \leq \operatorname{Tr} \, K_A^\dagger K_A.$$

With this restriction the determinant of $U_A \in \mathcal{M}'$ can be defined by using the standard renormalization prescription for determinants

$$\log \det' U = \sum_{i=1}^{\infty} d_i \log \frac{1+k_i}{e^{k_i}},$$

in terms of the eigenvalues of K_A , k_i , $i=1,2,\cdots$, and their degeneracies, d_i , $i=1,2,\cdots$. Finiteness of this prescription for the regularized determinant $\det' U$ follows from the Hilbert-Schmidt character of K_A which in particular implies a discrete spectrum with finite degeneracies satisfying the Hilbert-Schmidt condition $K_A^{\dagger}K_A = \sum_{i=1}^{\infty} d_i |k_i|^2 \leq \infty$.

The first Chern class of the regularized determinant bundle is given by the one form

$$\alpha = \frac{1}{2\pi} d \log \det'(\gamma(\theta)) \tag{5.2}$$

For any closed curve $\gamma: S^1 \to \mathcal{M}'$ in the self-adjoint grassmannian, we define its Maslov index $\nu_M(\gamma)$ as the winding number of the curve det $' \circ \gamma: S^1 \to U(1)$ [24], in other words,

$$\nu_M(\gamma) = \frac{1}{2\pi} \int_0^{2\pi} \partial_\theta \log \det'(\gamma(\theta)) d\theta.$$
 (5.3)

The Maslow index $\nu_M(\gamma)$ is the sum of the winding numbers of the maps $\lambda_i(\theta): S^1 \to U(1)$ described by the flow of eigenvalues of γ around U(1). By continuity of γ and compactness of S^1 it follows that only a finite number of eigenvalues reach the value $\lambda_i = -1$ for any value of $\theta \in [0, 2\pi)$. It is clear that the winding number of the map $\lambda_i(\theta)$ is measured by $\frac{1}{2\pi} \int_0^{2\pi} \partial_\theta \log(\lambda_i(\theta)) d\theta$ and also by the number of indexed crossings of the point $\lambda_i = -1$. By construction $\nu_M(\gamma)$ is the finite sum of the non-trivial winding numbers and is always an integer. This fact and the existence of curves with only one crossing through -1 implies that α is in the generating class of the cohomology group $H^1(\mathcal{M}', \mathbb{Z})$.

The subspace \mathcal{M}' of unitary operators of the form $U = \mathbb{1} + K$ has richer topological and geometrical structures. In particular we will see that it is a Grassmaniann, the selfadjoint Grassmannian.

It is obvious that the subspaces $\mathcal{M}_+ = L^2(\Gamma, \mathbb{C}^N) \times \{\mathbf{0}\} = \{ (\varphi, \mathbf{0}) \mid \varphi \in L^2(\Gamma, \mathbb{C}^N) \}$ and $\mathcal{M}_- = \{\mathbf{0}\} \times L^2(\Gamma, \mathbb{C}^N) = \{ (\mathbf{0}, \dot{\varphi}) \mid \dot{\varphi} \in L^2(\Gamma, \mathbb{C}^N) \}$ which correspond to Dirichlet and Neumann boundary conditions are isotropic in \mathcal{M} and they are paired by Σ . In fact,

$$\Sigma(\varphi_1, \mathbf{0}; \mathbf{0}, \dot{\varphi}_2) = -i \langle \varphi_1, \dot{\varphi}_2 \rangle_{\Gamma}$$

The block structure of Σ with respect to the isotropic polarization $\mathcal{M}_+ \oplus \mathcal{M}_-$ of \mathcal{M} reads

$$\Sigma = \begin{pmatrix} 0 & -i\langle .\,,.\,\rangle_{\Gamma} \\ i\langle .\,,.\,\rangle_{\Gamma} & 0 \end{pmatrix}.$$

Notice that in higher dimensions only the subspace $\mathcal{M}_{-} \subset \mathcal{M}$ belongs to \mathcal{M}' , $\mathcal{M}_{+} \cap \mathcal{M}' = \emptyset$.

The pseudo-hemitian structure Σ can be diagonized by means of the Cayley transform

$$C(\varphi, \dot{\varphi}) = (\phi^+, \phi^-) = (\varphi + i\dot{\varphi}, \varphi - i\dot{\varphi}). \tag{5.4}$$

which transforms Σ into

$$\Sigma_c = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}.$$

There is another canonical hermitian product on $\mathcal{M}_+ \oplus \mathcal{M}_-$ given by

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

which defines a Hilbert structure $\langle .,. \rangle$ on $\mathcal{M}_+ \oplus \mathcal{M}_-$.

The Grassmannian $Gr(\mathcal{M}_+, \mathcal{M}_-)$ of $L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$ is the infinite dimensional Hilbert manifold of closed subspaces W in $\mathcal{M}_+ \oplus \mathcal{M}_-$ such that the projection on the first factor $\pi_+: W \to \mathcal{M}_+$ is a Fredholm operator and the projection on the second factor $\pi_-: W \to \mathcal{M}_-$ is Hilbert–Schmidt, that is, $\operatorname{Tr} \pi_-^{\dagger} \pi_- < \infty$.

The selfadjoint Grassmaniann $Gr(\mathcal{M}_+, \mathcal{M}_-) \cap \mathcal{M}$ is defined by the selfadjoint extensions of Δ_A which belong to the Grassmaniann $Gr(\mathcal{M}_+, \mathcal{M}_-)$. This subspace might be considered as the space of mild self-adjoint extensions of Δ_A whose projection into the subspace \mathcal{M}_- is Hilbert-Schmidt. It is possible to see that the self-adjoint Grassmannian is a submanifold of the Grassmannian itself and can be identified with \mathcal{M}' the space of unitary operators of \mathcal{M} which are of the form $U = \mathbb{1} + K_A$. This follows from the fact that in some parametrization of \mathcal{M}'

$$\pi_{-} = \frac{iK_A}{2\sqrt{U}},\tag{5.5}$$

which implies that Tr $\pi_{-}^{\dagger}\pi_{-}=\frac{1}{4}$ Tr $K_{A}^{\dagger}K_{A}$, i.e. π_{-} is Hilbert-Schmidt if and only if K_{A} is Hilbert-Schmidt.

The intersection of the Cayley submanifold C_{\pm} with \mathcal{M}' defines a subspace of the self-adjoint Grassmannian $C'_{\pm} \subset \mathcal{M}'$ which has a stratified structure according to the number of eingenvalues ± 1 of the corresponding unitary operator, i.e.

$$\mathcal{C}'_{\pm} = \bigcup_{n=1}^{\infty} \mathcal{C}'_{\pm}^{n},$$

where $C_{\pm}^{'n} = \{U \in \mathcal{U}(L^2(\Gamma, \mathbb{C}^N); \pm 1 \in \sigma(U) \text{ with multiplicity } n\}$. Notice that the spectrum of unitary operators in the selfadjoint Grassmannian is discrete.

Given a continuous curve $\gamma:[0,1] \to \mathcal{M}'$ we define its Cayley index $\nu_c(\gamma)$ as the indexed sum of crossings of γ through the Cayley submanifold \mathcal{C}'_- (notice that the Cayley submanifolds \mathcal{C}'_+ are oriented). This is equivalent to the sum of anti-clockwise crossing

of eigenvalues of γ through the point -1 on the unit circle U(1) minus the sum of clockwise crossings weighted with the respective degeneracies. Therefore, the Cayley index $\nu_c(\gamma)$ of γ is equivalent to its Maslow index $\nu_M(\gamma)$ and we have the following theorem.

Theorem 4: The Maslow and Cayley indices of a closed curve γ in the selfadjoint Grassmannian are the same $\nu_M(\gamma) = \nu_c(\gamma)$. The Cayley manifold \mathcal{C}'_- is dual of the Maslow class α .

For any unitary operator $U \in \mathcal{M}$ we will define its degenerate dimension as the dimension of the eigenspace with eigenvalue -1. If U is in the self-adjoint Grassmaniann \mathcal{M}' the dimension of the eigenspace with eigenvalue -1 is finite and the degenerate dimension of the operator is finite. We shall denote such number by n(U). It is an indicator of the level of $\gamma(\theta)$ in statratification structure of \mathcal{C}' : $U = \gamma(\theta) \in \mathcal{C}'^n$ if and only if n(U) = n The Cayley index of any curve $\gamma \in \mathcal{M}'$ can be given in terms of this number by the expression

$$\nu_c(\gamma) = \int_0^{2\pi} \partial_\theta n(\gamma(\theta)) d\theta. \tag{5.6}$$

Since (5.6) is the integral of a pure derivative it vanishes unless there is a singularity in the integrand. This only occurs at the jumps of $n(\gamma(\theta))$ i.e. when one more eigenvalue of $U = \gamma(\theta)$ becomes equal to -1. $\nu_M(\gamma)$ is in fact a bookkeeping of the number of eigenvalues of $\gamma(\theta)$ that cross through -1 and since it is of bounded variation on \mathcal{M}' the integral in eq. (5.6) is always finite and gives the Cayley index. This construction provides an alternative (singular) characterization of the first Chern class of the determinant bundle $\det_{\mathcal{M}'}(\mathcal{M}', U(1))$ and the generating class of the first homology group $H^1(\mathcal{M}', \mathbb{Z})$ of \mathcal{M}' .

6. Topology change and edge states.

Although the operator $\Delta_A + 1$ is positive in $C_0^{\infty}(M, E)$ its selfadjoint extensions might not be definite positive. In fact, if the selfadjoint extension does not belong to any of the Cayley submanifolds \mathcal{C}_{\pm} it is easy to show by integration by parts that

$$(d \Psi_1, d \Psi_2) = (\Psi_1, \Delta_A \Psi_2) + (\varphi_1, \dot{\varphi}_2) = (\Psi_1, \Psi_2) + (\varphi_1, A\varphi_2) = (\Psi_1, \Delta_A \Psi_2) + (A^{-1}\dot{\varphi}_1, \dot{\varphi}_2),$$

where

$$(d \Psi_1, d \Psi_2) = \int_{\Gamma} d \Psi_1 \wedge *d \Psi_2,$$

and A is given by (5.4).

Thus, only if $(d \Psi, d \Psi) - (\varphi, A\varphi)$ for every Ψ is positive the operator Δ_A will be positive. In particular if the boundary operator A is positive it might occur that the whole operator Δ_A might loose positivity. The existence of negative energy levels is thus possible for some boundary conditions. It can be seen that the states which have negative energy are in a certain sense edge states.

Theorem 5: For any selfadjoint extension Δ_A^U of Δ_A whose unitary operator U has one eigenvalue -1 with smooth eigenfunction, the family of selfadjoint extensions of the form $U_t = Ue^{it}$ with $t \in (0, \pi/2)$, has for small values of t one negative energy level which corresponds to an edge state. The energy of this edge state becomes infinite when $t \to 0$.

Proof: Let $\xi \in L^2(\Gamma, \mathbb{C}^N)$ be a smooth eigenstate of U with eigenvalue -1. Then, $U_t \xi = \mathrm{e}^{it} \xi$. Let us consider Gaussian coordinates in a collar $\mathcal{C}_{\Gamma} \subset M$ around the boundary Γ of M. One of those coordinates is the "radius" r and the others can identified with boundary coordinates sifted inside the collar; i.e. $\mathcal{C}_{\Gamma} \approx [1 - \epsilon, 1] \times \Gamma$. In this coordinates the metric matrix looks like

$$g = \begin{pmatrix} 1 & 0 \\ 0 & \Omega(r, \Gamma) \end{pmatrix}. \tag{6.1}$$

We shall consider the following change of coordinates $r \leftrightarrow s$ with $s = \frac{\pi}{2\epsilon}(1-r)$.

If we extend the function ξ from the boundary Γ to an edge state Ψ in the bulk domain M by

$$\Psi(x) = \begin{cases} \xi(\Gamma)e^{-k \operatorname{tg} s} & x = (s, \Gamma) \in \mathcal{C} \\ 0 & x \notin \mathcal{C} \end{cases}, \tag{6.2}$$

it is easy to check that the extended function Ψ is smooth in M and for

$$k = \frac{2\epsilon}{\pi} \operatorname{ctg} \frac{t}{2}$$

belongs to the domain of the selfadjoint extension of $\Delta_A^{U_t}$ associated to the unitary matrix $U_t = e^{it}U$. Thus, we have

$$\left(\Psi, \Delta_A^{U_t} \Psi\right) = \left(d_A \Psi, d_A \Psi\right) - \operatorname{ctg} \frac{t}{2} \left(\xi, \xi\right) \tag{6.3}$$

where

$$(d_A \Psi, d_A \Psi) = \int_0^{\pi/2} ds \int_{\Gamma} d\mu_{\Gamma}(s) |\xi|^2 (\frac{k^2 \pi}{2\epsilon}) (1 + (\operatorname{tg} s)^2)^2 e^{-2k \operatorname{tg} s} + \frac{2\epsilon}{\pi} \int_0^{\pi/2} ds \int_{\Gamma} d\mu_{\Gamma}(s) (\xi^*, \Delta_{\Gamma} \xi) e^{-2k \operatorname{tg} s}.$$
(6.4)

For small enough $\epsilon << 1$ we have that the dependence on s of Ω might be negligible $|\Omega(s,\Gamma)| < |\Omega(0,\Gamma)|(1+\delta)$. Thus,

$$(d_A \Psi, d_A \Psi) < \left(\frac{k}{2} + \frac{1}{4k}\right) \frac{\pi(1+\delta)}{2\epsilon} \|\xi\|^2 + \frac{2\epsilon(1+\delta)}{\pi} (\xi^*, \Delta_{\Gamma} \xi)$$
 (6.5)

and

$$\left(\Psi, \Delta_A^{U_t} \Psi\right) < \frac{\pi}{2\epsilon} \left(\frac{1}{4k} (1+\delta) - \frac{k}{2} (1-\delta)\right) \|\xi\|^2 + \frac{2\epsilon (1+\delta)}{\pi} (\xi^*, \Delta_{\Gamma} \xi), \tag{6.6}$$

which shows that $\left(\Psi, \Delta_A^{U_t} \Psi\right) < 0$ is not positive for small values of $\varphi = 2 \operatorname{arc} \operatorname{ctg} \left(k\pi/2\epsilon\right)$. Notice that the normalization of the edge state Ψ

$$||\Psi||^2 = \int_M (\Psi^{\dagger}, \Psi)_x \, d\mu_g(x) \ge \frac{\pi (1 - \delta)}{2\epsilon} \, ||\xi||^2 \int_0^{2\pi} ds \, e^{-2k \operatorname{tg} s}$$

vanishes in the limit $t \to 0$ but it is always a positive factor for $t \neq 0$ which preserves the bound (6.6). Moreover, the nature of the edge state Ψ also shows the existence of a ground state Ψ_0 with negative energy which is an edge state. The energy E_0 of this state goes to $-\infty$ as $t \to 0$, whereas the edge state Ψ_0 schrinks to the edge disappearing from the spectrum of $\Delta_A^{U_t}$ in that limit.

Although the role of boundary conditions in the two Cayley submanifold C_{\pm} is quite similar from the mathematical point of view the boundary conditions are quite different from the physical viewpoint. In particular, an analysis along the lines of the proof of the above theorem leads to the same (6.6) inequality but with

$$k = \frac{2\epsilon}{\pi} \operatorname{tg} \frac{t}{2}$$

which points out the existence of edge states with very large (positive) energy as $t \to 0$). It can also be shown that in that limit one energy level crosses the zero energy level becoming a zero mode of the Laplacian operator. Therefore, the role of boundary conditions in C_{-} (e.g. Dirichlet) is very different of that of boundary conditions in C_{+} (e.g. Newmann).

Notice that the result of the theorem does not require U to be in the selfadjoint Grassmannian \mathcal{M}' . This is specially interesting, because there is a very large family of boundary conditions which do not belong to \mathcal{M}' . In particular, boundary conditions implying a topology change in higher dimensions are not in \mathcal{M}' because the corresponding unitary operators in $\mathcal{U}(\Gamma)$ present an infinity of eigenvalues ± 1 which implies that U

cannot be of the form $\mathbb{1} + K$ with K Hilbert-Schmidt. Indeed, all boundary conditions which involve a change of topology, i.e. gluing together domains \mathcal{O}_1 , \mathcal{O}_2 of the boundary Γ , belong to $\mathcal{C}_- \cap \mathcal{C}_+$. This property follows from the fact that the boundary conditions imply that the boundary values $\varphi, \dot{\varphi}$ are related in the domains that are being glued together, i.e. $\varphi(\mathcal{O}_1) = \varphi(\mathcal{O}_2), \dot{\varphi}(\mathcal{O}_1) = -\dot{\varphi}(\mathcal{O}_2)$, respectively. These requirements imply that the unitary operator U corresponding to this boundary condition is identically $U = \mathbb{1}$ on the subspace of functions such that $\varphi(\mathcal{O}_1) = \varphi(\mathcal{O}_2)$ and $U = -\mathbb{1}$ on the subspace of functions such that $\varphi(\mathcal{O}_1) = -\varphi(\mathcal{O}_2)$. Since both subspaces are infinite-dimensinal for manifolds M with more that one dimension it is clear that those operators U do not belong to $\mathcal{C}'_- \cap \mathcal{C}'_+$. However the result of Theorem 5 implies that there always exists a boundary condition close to one involving the gluing of the domains with very large negative energy levels. This means that Cayley manifold $\mathcal{C}_- \cap \mathcal{C}_+$ is also very special and that topology change involves an interchange of an infinite amount of quantum energy. The result might have relevant implications in quantum gravity and string theory.

7. Conclusions

We have not analysed asymptotic boundary conditions which appear in singular boundary problems like a particle moving in a Dirac delta potential in the plane [25] or in the asymptotic Minkowskian boundary of anti-deSitter space-times. The later is of relevant interest in the analysis of the Maldacena conjecture [16]. However, if we regularize the boundary we can use the standard boundary conditions discussed throught the paper and consider some renormalization group flow limit which keep the selfadjoint character of the Laplace-Beltrami operator. Another interesting boundary effects which are not analysed in this paper are the deformation of the boundary and the inclusion of local insertions. In two dimensions, both effects are connected with theory of integrable systems (see Refs. [26][27])

For smooth boundaries we have given a very simple characterization of the self-adjoint extensions of the covariant Laplacian in terms of boundary data, which although equivalent to von Neumann's characterization based on deficiency index spaces, is more convenient for physical applications. The space of all boundary conditions exhibits a natural group structure and a non-trivial topology. In this space processes involving topology change can be naturally described. Boundary conditions involving topology change can describe in the same scenario open and closed strings and smooth interpolations between both type

of strings. This might be relevant for new developments in string theory. We have shown that for any adiabatic change of boundary conditions which involves a crossing of the Cayley submanifold \mathcal{C}_{-} there is an edge state which becomes an infinite negative energy level at the boundary condition on \mathcal{C}_{-} . Negative energy states are only possible if they are localized near the the boundary (edge states). The number of crossings of \mathcal{C}_{-} for any closed loop γ of boundary conditions defines a Maslov index $c_{M}(\gamma)$ which identifies with the generator of the first cohomology group of the space of all boundary conditions $H^{1}(\mathcal{M}', \mathbb{Z})$.

In the case of the Cayley submanifold C_+ a similar argument shows that for any one-parameter family of boundary conditions which intersects at the Cayley submanifold C_+ there is one energy level of the Δ_A which becomes a zero level state on the Cayley submanifold.

From the physical point of view the above results show that the boundary has a contribution to the energy levels and some of those energy levels are rather localized at the edge of the boundary (edge states). For boundary conditions which approach a topology changing boundary condition at least one energy level acquires a very large negative energy which means that such a transition from the energetic point of view is singular. However, looking at any time to the corresponding boundary condition no singularity is shown in the spectrum because those states which become highly energetic also become very singular and disappear from the domain of the selfadjoint operator and consequently their energy levels from the spectrum. However, the effect leads to some observable phenomena. For instance, the dependence of Casimir energy on the boundary conditions for a scalar field becomes singular when the boundary condition approaches a boundary condition with unitary operators with extra -1 eigenvalues. In particular, this occurs for boundary conditions involving a topology change which might have relevant implications for quantum gravity and string theory.

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Appendix A. Topology Change and One Dimensional Boundary Conditions

To illustrate the utility of the above geometric approach we consider some simple applications to Sturm-Liouville problems. In such a case the configuration space is constrained to an interval M = [0,1] of real numbers. The metric g is the standard Euclidean metric of \mathbb{R} and the symmetric operator is the Sturm-Liouville second order differential operator

$$\mathbb{H} = \frac{1}{2}\Delta = -\frac{1}{2}\frac{d}{dx^2}$$

defined on $C_0^{\infty}([0,1])$. The boundary set is in this case discrete $\partial\Omega = \{0,1\}$ and $L^2(\partial\Omega) = \mathbb{C}^2$. Therefore the different selfadjoint extension are parametrized by a 2×2 unitary matrix

$$U = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} \tag{A.1}$$

The domain of the associated extension is given by the functions of $L^2([0,1])$ whose boundary values satisfy the following equations,

$$\begin{pmatrix} \varphi(0) + i\dot{\varphi}(0) \\ \varphi(1) + i\dot{\varphi}(1) \end{pmatrix} = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} \begin{pmatrix} \varphi(0) - i\dot{\varphi}(0) \\ \varphi(1) - i\dot{\varphi}(1) \end{pmatrix}, \tag{A.2}$$

where $\dot{\varphi}(0) = \varphi'(0)$ y $\dot{\varphi}(1) = -\varphi'(1)$.

Some specially interesting examples correspond to the case when the matrix U is diagonal or anti-diagonal. In the first case we have

$$U = \begin{pmatrix} e^{i\epsilon} & 0\\ 0 & e^{i\gamma} \end{pmatrix} \tag{A.3}$$

which corresponds to the boundary conditions

$$-\sin\frac{\epsilon}{2}\varphi(0) + \cos\frac{\epsilon}{2}\dot{\varphi}(0) = 0$$

$$-\sin\frac{\gamma}{2}\varphi(1) + \cos\frac{\gamma}{2}\dot{\varphi}(1) = 0$$
 (A.4)

which includes Newmann $\dot{\varphi}(0) = \dot{\varphi}(1) = 0$ and Dirichlet $\varphi(0) = \varphi(1) = 0$ boundary conditions. In the *anti-diagonal* case

$$U = \begin{pmatrix} 0 & e^{-i\epsilon} \\ e^{i\epsilon} & 0 \end{pmatrix} \tag{A.5}$$

we have (pseudo)periodic boundary conditions

$$\varphi(1) = e^{i\epsilon} \varphi(0)$$

$$\varphi'(1) = e^{i\epsilon} \varphi'(0)$$
(A.6)

 $\varphi(1) = e^{i\epsilon}\varphi(0)$ with probability flux propagating through the boundary. This condition is in fact a topological boundary condition which corresponds to the folding the interval into a circle S^1 , with a magnetic flux ϵ crossing throughout.

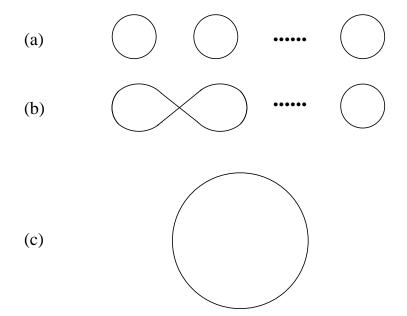


Figure 1. Boundary conditions for a family of disconected intervals in \mathbb{R} might correspond to different topologies. In case (a) we have N disconnected circles. In case (b) two circles merge into an eight. The last case (c) corresponds to a single circle. Generic boundary conditions describe N open disconnected strings

If we have several disconnected intervals $M = \bigcup_{i=1}^{N} [a_i, b_i]$ then the space of boundary conditions is given by U(2N). If we identify some of the boundaries with opposite orientations we can generate different closed manifolds with $r \leq N$ circle components. The corresponding operators go from

$$U_1 = \begin{pmatrix} 0 & \mathbb{1}_N \\ \mathbb{1}_N & 0 \end{pmatrix} \tag{A.7}$$

for the connected manifold, till

$$U_N = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$
(A.8)

the manifold made of N disconnected circles (see Fig. 1). Therefore, in U(2N) it is possible to describe an smooth transition from one topology to the other, which provides a theoretical framework for topological transitions [14], in particular, for a joint description of open and closed strings.

Appendix B. Higher dimensional boundary conditions.

The last type of boundary condition can be generalized for arbitrary dimensions. Let us first consider the 2-dimensional disk $D = \{x \in \mathbb{R}^2; ||x|| \leq 1\}$. The space of all boundary conditions of the laplacian can then be identified with $\mathcal{U}(L^2(S^1))$ which in this case is an infinite dimensional group. Examples of selfadjoint extensions include Dirichlet U = -1 and Neumann U = 1 boundary conditions. There are other boundary conditions which correspond to topological foldings of the disk into Riemann surfaces any genus. Let us first consider the case of the sphere S^2 .

$$\partial_{\theta}\varphi = 0$$

$$\int_{S^{1}} \dot{\varphi} \, d\mu_{\Gamma} = 0 \tag{B.1}$$

The associated unitary operator is

$$U_0 = \begin{pmatrix} P_0 & 0\\ 0 & \mathbb{1} - P_0 \end{pmatrix} \tag{B.2}$$

where

$$P_0 = \frac{1}{2\pi} \int_{S^1} \cdot d\theta$$

is the projector to the constant functions subspace $\mathcal{H}_0 = \{\varphi \in L^2(S^1); \partial_\theta \varphi = 0\}$ of $L^2(S^1)$ and we have split $L^2(S^1)$ into \mathcal{H}_0 and its orthogonal complement \mathcal{H}_0^{\dagger} . The selfadjoint extension U_0 corresponds to the topology of the sphere S^2 .

It is obvious how to generalize the above construction for higher genus. For genus 1 surfaces we decompose the boundary S^1 into its four quadrants $I_1 = [0, \pi/2]$, $I_2 = (\pi/2, \pi)$, $I_3 = [\pi, 3\pi/2]$ and $I_4 = (3\pi/2, 2\pi)$ and identify the points $\theta \in I_1$ with $3\pi/2 - \theta \in I_3$, and the points $\theta' \in I_2$ with $5\pi/2 - \theta' \in I_4$. If we split $L^2(S^1) = \bigoplus_{r=1}^4 L^2(I_r)$ into its components over the four quarters of S^1 . The corresponding selfadjoint extension is given by the U(8)unitary operator

$$U_1 = \begin{pmatrix} 0 & 0 & \mathbb{1}_2 & 0 \\ 0 & 0 & 0 & \mathbb{1}_2 \\ \mathbb{1}_2 & 0 & 0 & 0 \\ 0 & \mathbb{1}_2 & 0 & 0 \end{pmatrix}$$
 (B.3)

defines the quantum selfadjoint extension of \mathbb{H} which corresponds to toroidal compactification of M.

Other splittings of the circle give rise to different tori, but for all of them it is necessary to have an isometry between the pairs of alternating arcs.

For arbitrary genus g, we have the straightforward generalization, via an splitting of the circle S^1 into 2g+2 arcs. The unitary operator

$$U_g = \begin{pmatrix} 0 & \mathbb{1}_{2g+2} \\ \mathbb{1}_{2g+2} & 0 \end{pmatrix}. \tag{B.4}$$

In this way all possible string world sheets transitions can be described in the set of boundary conditions $\mathcal{U}(L^2(S^1))$ in a smooth set up. If we substitute the identity operators $\mathbb{1}_N$ by diagonal phases the boundary condition describes the effect of magnetic fluxes crossing though the handles of the compact surface of genus g. Moreover the creation and annihilation of bubbles, baby universes and transition between them can also be described by considering families of disks in analogy with the one-dimensional case of Appendix A.

Many of those boundary conditions involving non-trivial topological foldings can be generalized for the higher dimensional case. However much more conditions associated to different topological manifolds appear. The simplest one is the corresponding to the folding of the n-dimensional ball to the n-dimensional sphere S^n . The corresponding unitary operator is given by

$$U_{S^n} = \begin{pmatrix} P_0 & 0\\ 0 & P_0 - 1 \end{pmatrix} \tag{B.5}$$

where as in the one-dimensional case

$$P_0 = \frac{1}{2\pi} \int_{S^n} \cdot d\mu_{S^n}$$

denotes the projector to the subspace of constant functions $\mathcal{H}_0 = \{ \varphi \in L^2(S^n); d\varphi = 0 \}$ and $L^2(S^n) = \mathcal{H}_0 \oplus \mathcal{H}_0^{\dagger}$ has been split into \mathcal{H}_0 and its orthogonal complement \mathcal{H}_0^{\dagger} .

The common feature of all these boundary conditions involving topology change is that the unitary matrix have pairs of eigenvalues (1, -1) indicating that all of them belong to the Cayley manifold $\mathcal{C}_- \cap \mathcal{C}_+$.

Another type of boundary conditions can appear from the choice

$$U = \frac{\mathbb{1} \pm i\Delta_{\Gamma}}{\mathbb{1} \mp i\Delta_{\Gamma}}.$$

In this case $\varphi = \pm \Delta_{\Gamma} \dot{\varphi}$, and

$$(d \Psi_1, d \Psi_2) = (\Psi_1, \Psi_2) \pm (\varphi_1, \Delta_{\Gamma} \varphi_2).$$

we might have negative energy levels. In the presence of magnetic field a similar boundary condition leads to negative energy edge levels which are also present in the Hall effect in a Corbino disk [12].

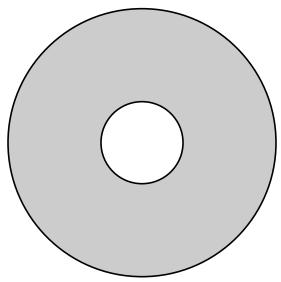


Figure 2. The Corbino disk.

Appendix C. Self-Adjoint Extensions of Higher Order Operators.

The theory of selfadjoint extensions of Laplace-Beltrami operators developed throughout the paper can be generalized in a straightforward way for other differential operators like the Dirac operator \mathcal{D}_A [28] and different powers and products of \mathcal{D}_A and Δ_A^2 . To illustrate how this can be achieved let us consider for simplicity the forth order differential operator given by the square of the covariant Laplace-Beltrami Δ_A^2 . Some of boundary conditions of Δ_A^2 are induced by those of Δ_A , but the space of boundary conditions of the square operator is much larger.

The operator Δ_A^2 is symmetric on $C_0^{\infty}(M, E)$ with respect to the hermitian product $\langle ., . \rangle$ of E defined by (2.1), but in order to obtain a selfadjoint extension we have to define a larger domain where the boundary terms arising from the integration by parts formula

$$\langle \psi_1, \Delta_A^2 \psi_2 \rangle = \langle \Delta_A^2 \psi_1, \psi_2 \rangle + i \Sigma_2 (\psi_1, \psi_2), \qquad (C.1)$$

vanish. This boundary term

$$\Sigma_{2}(\psi_{1}, \psi_{2}) = i \int_{M} d\left[(*d_{A}\psi_{1}, \Delta_{A}\psi_{2}) + (*d_{A}\Delta_{A}\psi_{1}, \psi_{2}) - (\Delta_{A}\psi_{1}, *d_{A}\psi_{2}) - (\psi_{1}, *d_{A}\Delta_{A}\psi_{2}) \right]$$

only really depends on the boundary values $\varphi, \dot{\varphi}, \Delta_A \varphi, \dot{\Delta_A} \varphi$ defined by

$$\varphi_i = j^* \psi_i, \ \dot{\varphi}_1 \ d\mu_{\Gamma} = j^* [*d_A \psi_i]; \ \Delta_A \varphi_i = j^* [\Delta_A \psi_i], \ \Delta_A^{\dot{}} \varphi_i \ d\mu_{\Gamma} = j^* [*d_A \Delta_A \psi_i],$$

for i=1,2, because by Stokes theorem,

$$\Sigma_{2}(\psi_{1}, \psi_{2}) = i \int_{\Gamma} j^{*} \left[(*d_{A}\psi_{1}, \Delta_{A}\psi_{2}) + (*d_{A}\Delta_{A}\psi_{1}, \psi_{2}) - (\Delta_{A}\psi_{1}, *d_{A}\psi_{2}) - (\psi_{1}, *d_{A}\Delta_{A}\psi_{2}) \right]$$
$$= i \int_{\Gamma} \left[(\dot{\varphi}_{1}, \Delta_{A}\varphi_{2}) + (\dot{\Delta_{A}}\varphi_{1}, \varphi_{2}) - (\varphi_{1}, \dot{\Delta_{A}}\varphi_{2}) - (\Delta_{A}\varphi_{1}, \dot{\varphi}_{2}) \right] d\mu_{\Gamma}.$$

Again this boundary term $\Sigma_2(\psi_1, \psi_2)$ measures the net probability flux across the boundary. If the operator Δ_A^2 were self-adjoint this flux would have to be balanced or in other words, $\exp it\Delta_A^2$ would be an unitary operator and the probability preserved.

The different self-adjoint extensions of Δ_A^2 will be defined in the linear dense subspaces of $L^2(M,\mathbb{C}^N)$ containing $C_0^{\infty}(M,E)$ where the boundary term Σ_2 vanishes. They are therefore characterized by the maximal isotropic subspaces of the boundary data space

$$[L^2(\Gamma, \mathbb{C}^N)]^4 \times [L^2(\Gamma, \mathbb{C}^N)]^4 = \{(\varphi_1, \Delta_A \varphi_1, \dot{\varphi}_1, \dot{\Delta_A} \varphi_1); (\varphi_2, \Delta_A \varphi_2, \dot{\varphi}_2, \dot{\Delta_A} \varphi_2)\}$$

with respect to the pseudo-hermitian structure Σ_2 .

They are easier characterized after a double Cayley transform

$$C: [L^2(\Gamma, \mathbb{C}^N)]^4 \times [L^2(\Gamma, \mathbb{C}^N)]^4 \longrightarrow [L^2(\Gamma, \mathbb{C}^N)]^4 \times [L^2(\Gamma, \mathbb{C}^N)]^4$$

is performed

$$C\left((\varphi_{1},\dot{\varphi}_{1},\ \Delta_{A}\varphi_{1},\dot{\Delta_{A}}\varphi_{1}),(\varphi_{2},\dot{\varphi}_{2},\Delta_{A}\varphi_{2},\dot{\Delta_{A}}\varphi_{2})\right)$$

$$=\left((\phi_{1}^{+},\phi_{1}^{-},\Delta_{A}\phi_{1}^{+},\Delta_{A}\phi_{1}^{-}),(\phi_{2}^{+},\phi_{2}^{-},\Delta_{A}\phi_{2}^{+},\Delta_{A}\phi_{2}^{-})\right)$$

$$=\left((\varphi_{1}+i\dot{\Delta_{A}}\varphi_{1},\varphi_{1}-i\dot{\Delta_{A}}\varphi_{1},\Delta_{A}\varphi_{1}+i\dot{\varphi}_{1},\Delta_{A}\varphi_{1}-i\dot{\varphi}_{1}),\right)$$

$$(\varphi_{2}+i\dot{\Delta_{A}}\varphi_{2},\varphi_{2}-i\dot{\Delta_{A}}\varphi_{2},\Delta_{A}\varphi_{2}+i\dot{\varphi}_{2},\Delta_{A}\varphi_{2}-i\dot{\varphi}_{2})\right),$$
(C.2)

because the maximal isotropic spaces with respect to the transformed product

$$\Sigma_{2}^{c} \left((\phi_{1}^{+}, \phi_{1}^{-}, \Delta_{A} \phi_{1}^{+}, \Delta_{A} \phi_{1}^{-}), (\phi_{2}^{+}, \phi_{2}^{-}, \Delta_{A} \phi_{2}^{+}, \Delta_{A} \phi_{2}^{-}) \right)$$

$$= \langle \phi_{1}^{+}, \phi_{2}^{+} \rangle - \langle \phi_{1}^{-}, \phi_{2}^{-} \rangle + \langle \Delta_{A} \phi_{1}^{+}, \Delta_{A} \phi_{2}^{+} \rangle - \langle \Delta_{A} \phi_{1}^{-}, \Delta_{A} \phi_{2}^{-} \rangle.$$
(C.3)

are in one-to- one correspondence with the space of unitary operators

$$U\left(L^2(\Gamma,\mathbb{C}^N)\times L^2(\Gamma,\mathbb{C}^N)\right)$$

of the boundary space $L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$. Therefore, we have proved the following result.

Proposition: The set of self-adjoint extensions of Δ_A^2 is in one-to-one correspondence with the group of unitary operators of $L^2(\Gamma, \mathbb{C}^N) \times L^2(\Gamma, \mathbb{C}^N)$. The subgroup of unitary operators of the form $\mathbf{U} = (U, U)$ with $U \in L^2(\Gamma, \mathbb{C}^N)$ correspond to the boundary conditions induced by those of the second order operator Δ_A .

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